Single stage unit operations: flash

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Agenda

- Vapor-liquid equilibria
- Relative volatility
- Bubble point and dew point calculations
- Flash calculation
- Flash unit operation in Aspen+

Equilibrium ratio and relative volatility

- VLE in summary

0 < P < 2 bar $$Py_i = P_i^{sat}\gamma_i x_i$$

2 < P < 40 bar $$\varphi_i^V P y_i = \varphi_i^{*V,sat} P_i^{sat}\gamma_i x_i$$

P > 40 bar $$\varphi_i^V y_i = \varphi_i^L x_i$$

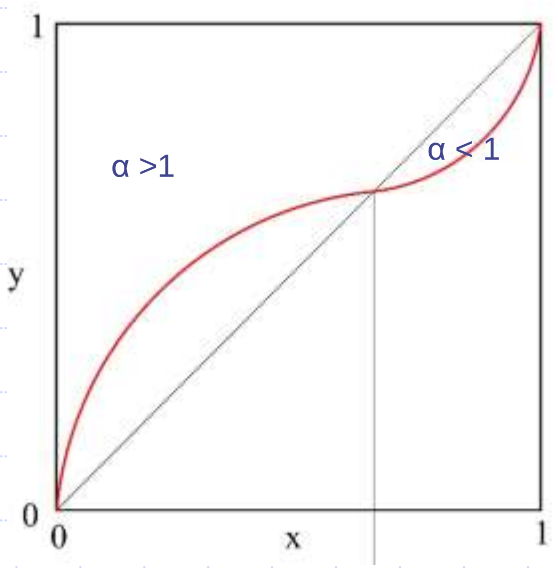
1. Equilibrium ratio (capacity factor): $$K_i = \frac{y_i}{x_i}$$
2. Relative volatility (selectivity): $$\alpha_{i,j} = S_{i,j} = \frac{K_i}{K_j}$$
3. For a binary system: $$\alpha = \alpha_{1,2} = \frac{y/x}{(1-y)/(1-x)}$$

Equilibrium ratio and relative volatility

- At low pressure

$$P y_i = P_i^{sat} \gamma_i x_i \qquad K_i = \frac{P_i^{sat}\gamma_i}{P} \qquad \alpha_{i,j} = \frac{K_i}{K_j} = \frac{P_i^{sat}(T)\gamma_i(T,x)}{P_j^{sat}(T)\gamma_j(T,x)}$$

- Relative volatility is NOT constant, depends on composition
  - *For ideal solution is nearly constant



At the azeotrope: $x = y \longrightarrow \alpha = 1$

Binary systems: Brown's equation

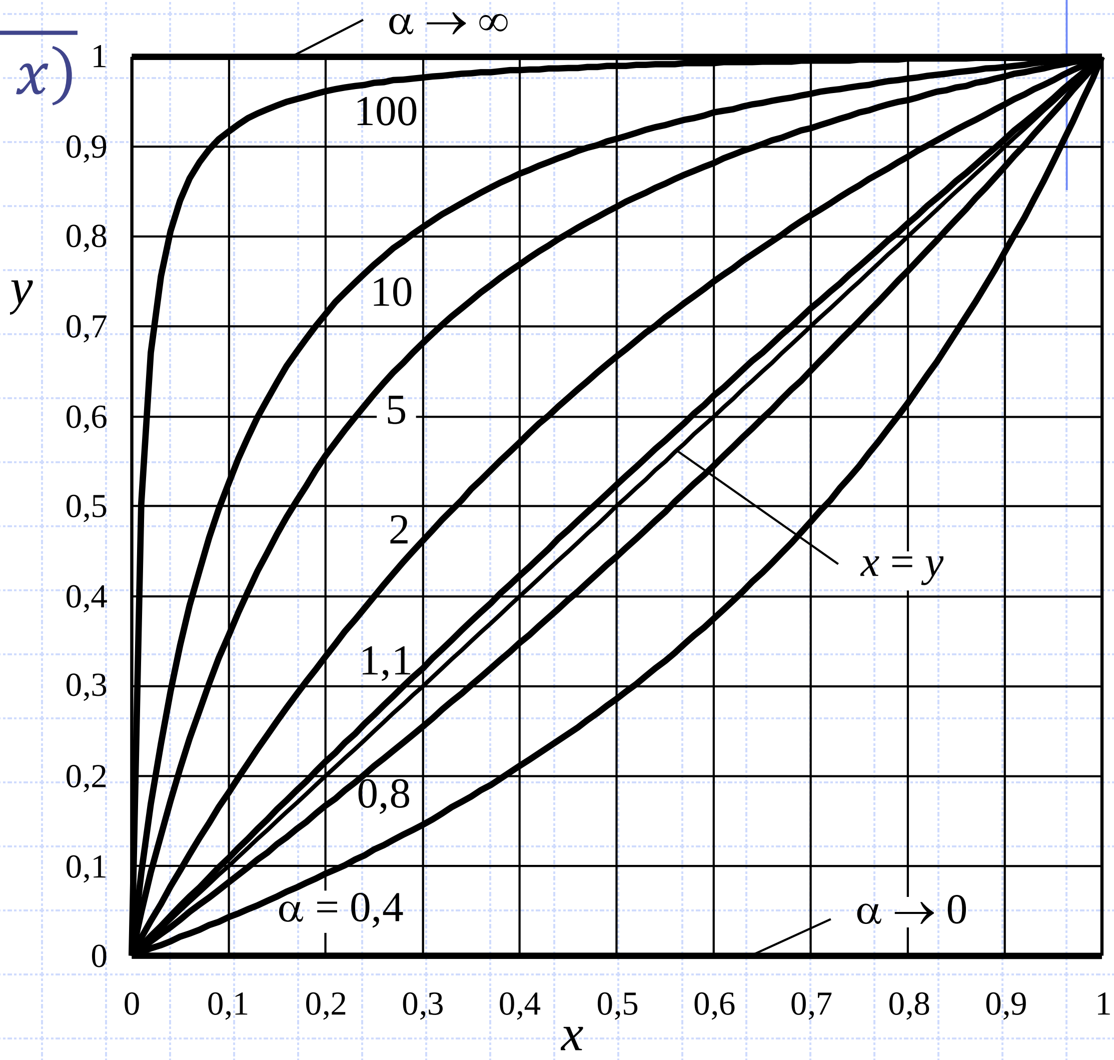
$$\alpha = \alpha_{1,2} = \frac{y/x}{(1-y)/(1-x)}$$

- Rearranging

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

- Limit for thermal separation processes

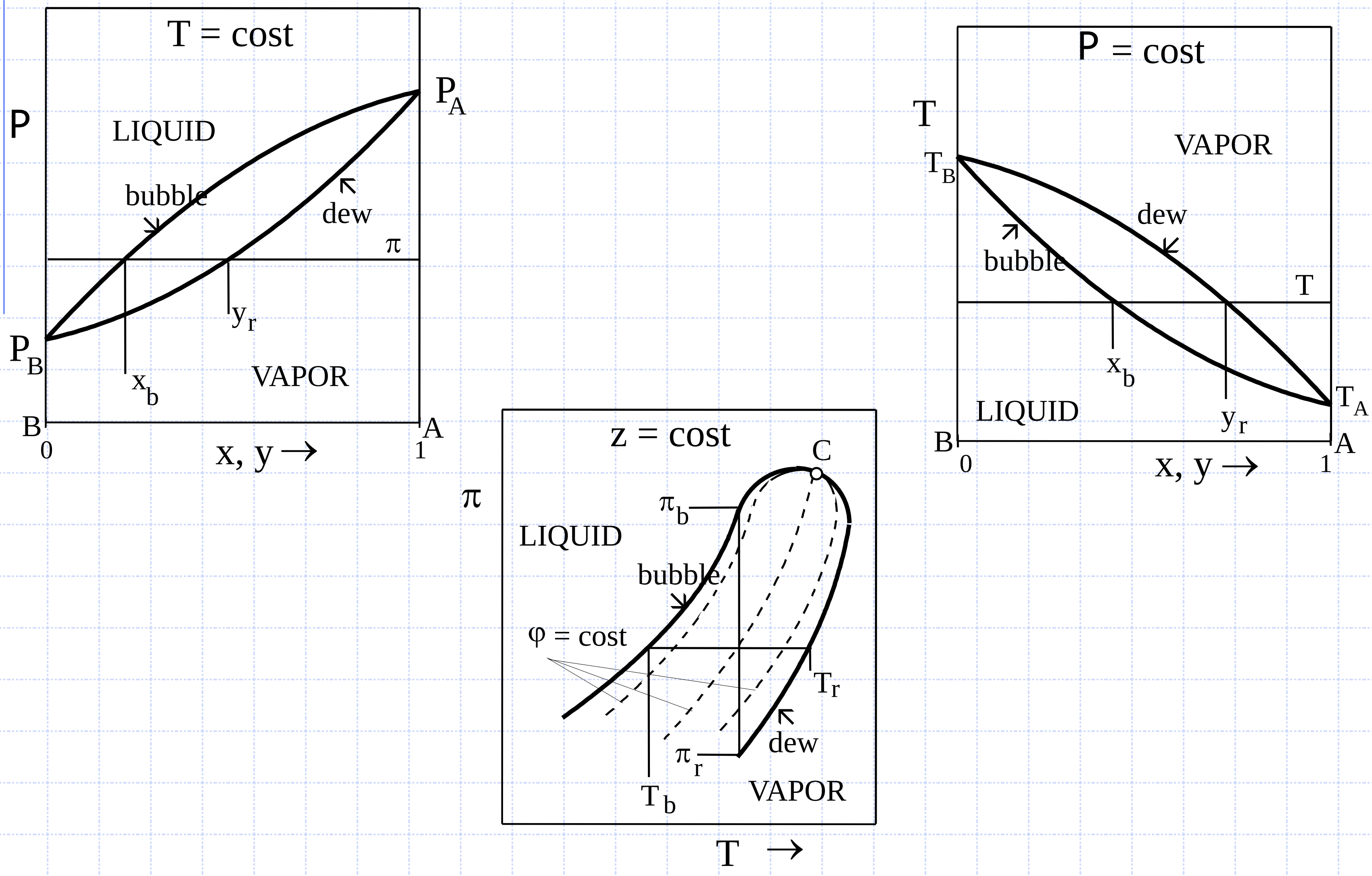
$$|\alpha_{i,j} - 1| \geq 0.05$$



Vapor liquid equilibrium calculation types

- Bubble point calculation,
  - *Given:* the liquid composition (x) and equilibrium T or P
  - *Calculate*: the vapor composition (y) and equilibrium P or T
- Dew point calculations
  - *Given:* the vapor composition (y) and equilibrium T or P
  - *Calculate*: the liquid composition (x) and equilibrium P or T
- Flash calculation
  - *Given:* the global composition (z) and equilibrium T and P
  - *Calculate*: the liquid (x) and vapor (y) compositions

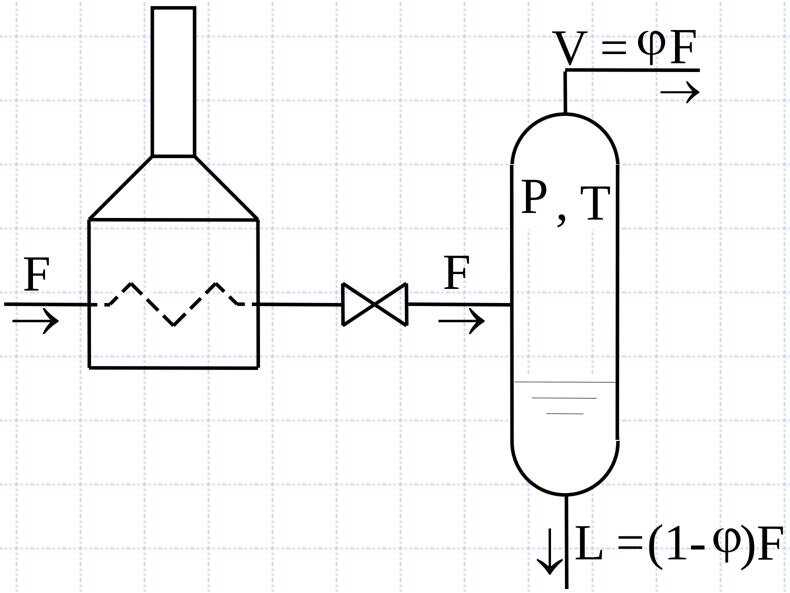
Vapor-Liquid Equilibrium Binary Systems

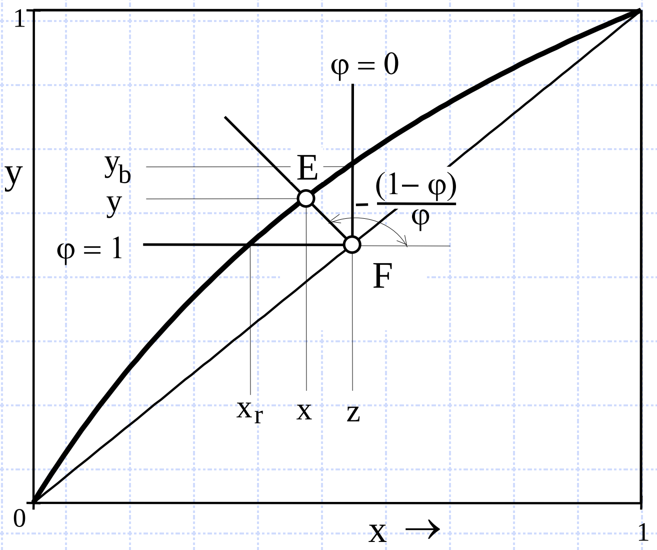


Bubble point and dew point calculations

- For a binary system:
  - Unknowns: T, P, x_1, x_2, y_1, y_2
  - Equilibrium equations: 2 isofugacity criteria
  - Summation of mole fractions: 2 equations
  - If two indipendent variables are fixed (P,x) two dependent variables are calculated (T,y)
  - The equations to be solved are the isofugacity criterion for two components in two phases
- For multicomponent systems:
  - Unknowns: T, P, x_i, y_i
  - Equlibrium equations: n isofugacity criterion
  - Summation of mole fractions: 2 equations
  - If n+1 (composition and P) is fixed, n+1 variables may be calculated (T and y_i)
  - The equations to be solved are the isofugacity criterion for n components in 2 phases

Single stage operation (Flash, mixer-settler,..)



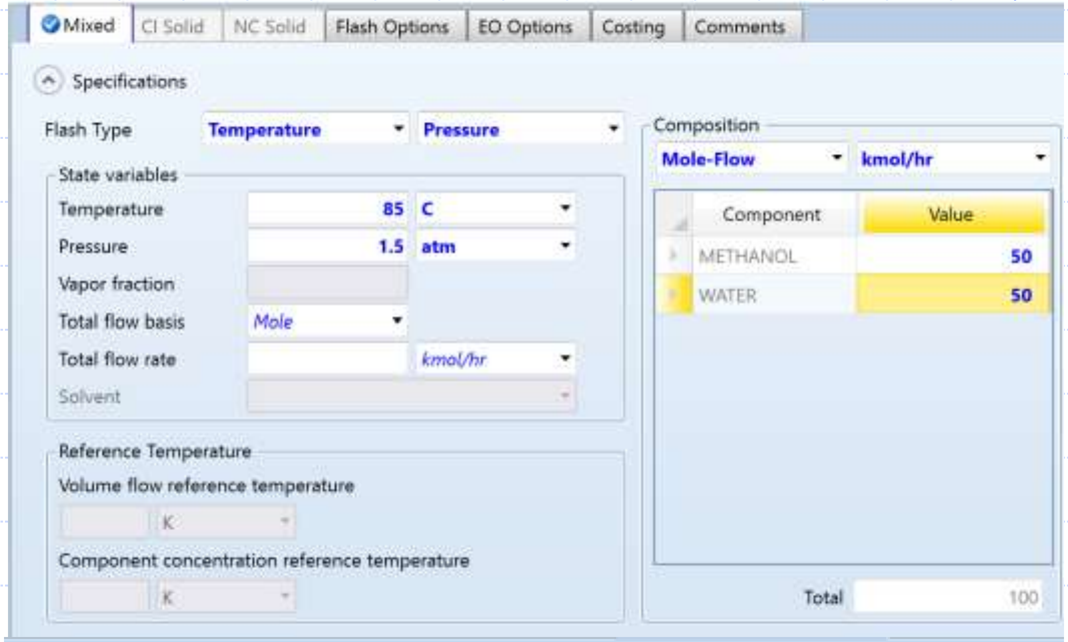


FLASH calculation

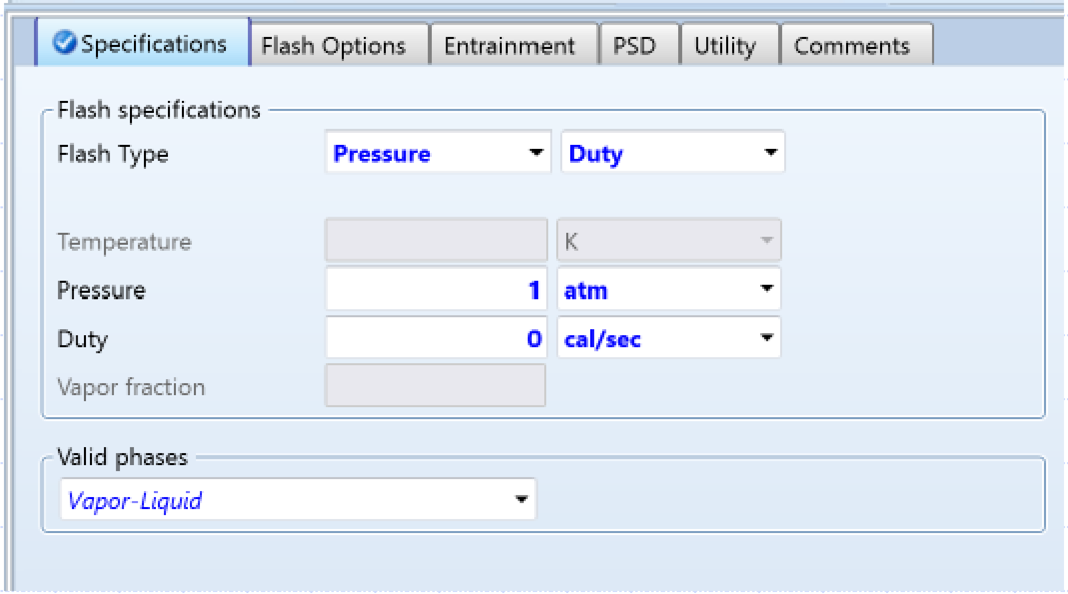
- For a binary system and isothermal flash:
  - Unknowns: T, P, F, z_1, z_2, V, L, x_1, x_2, y_1, y_2 (11)
  - Material balance equations: 2 chemical species
  - Equilibrium equations: 2 isofugacity criteria
  - Summation of mole fractions: 3 equations
  - If z_1, F, T and P is specified, the problem is solved for z_2, x_1, x_2, y_1, y_2, L, V
- For a multicomponent system and isothermal flash:
  - Unknowns: T, P, F, z_i, V, L, x_i, y_i (3(n-1) +5) = 3n+2
  - Material balance equations (n)
  - Equilibrium equations (n)
  - TOTAL Equations= 2n
  - IF z_i, F, T and P is specified (n-1+3)= n+2 → the problem is solved

Flash in Aspen+

- Input stream 1:
  - water – methanol
  - T=85°
  - P=1.5 atm
  - Mole flow 50 – 50 kmol/hr



- Block Flash input
  - Pressure = 1 atm
  - Duty = 0



Flash in Aspen+: results